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This is a summary of the results during the first year of a research program aimed at studying the atomic structure of semiconductor surfaces using scanning tunneling microscopy (STM). This research has concerned epitaxial growth of metals on the (111) and the (100) surfaces of silicon, with particular emphasis on the Si(100) surface. We have studied In, Sn, and Sb on Si(100), and Au on Si(111), focusing on phenomena such as order and disorder in surface reconstructions, nucleation and growth, growth anisotropy, and rearrangement of the Si substrate step distribution.

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Technical Performance Report

October 1, 1989 - September 30, 1990

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C. F. Quate

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Introduction

This is a brief summary of the results during the first year of a three year research program aimed at studying the atomic structure of semiconductor surfaces using scanning tunneling microscopy (STM). This research has concerned epitaxial growth of metals on the (111) and the (100) surfaces of silicon, with particular emphasis on the Si(100) surface. We have expanded our previous work on Si(100) by studying several different adsorbates, and also by looking at behavior at elevated temperatures. Studies of Al and In provide a natural extension of our work on Ga:Si(100) surfaces. These group III metals are important dopant materials in Si molecular beam epitaxy (MBE), and the determination of the dopant stabilized surface structures that arise have a bearing on the understanding of dopant incorporation during MBE. In a similar vein, we have also studied the Sb-terminated Si(100) surface. In addition to the fact that these surfaces all involve dopant species, these studies also lay the ground work for future efforts in examining the growth of III-V materials on Si(100).

Comparative studies of different metals on the Si(100) surface have shown that there is a common growth mode at room temperature for the group III metals Al, Ga, and In, as well as the group IV element Sn. At elevated temperatures, the behaviors of these metals diverge, with each inducing different reconstructions of the surface. In addition to the ordered surface reconstructions, effects such as anisotropic island growth, rearrangement of the Si substrate step distribution, and differing long range and short range order are seen in these various systems. Many of these phenomena are being observed for the first time on an atomic scale as a result of these STM studies.

In addition to the work on Si(100), we have carried out a detailed study of the Au/Si(111) system, focusing not only on the ordered surfaces that arise, but also on the nature of the phase transitions that occur as a function of Au coverage. As it turns out, the transition between the $\sqrt{3}\times\sqrt{3}$ and the 6x6 phases is unique in that it involves an evolution of the $\sqrt{3}\times\sqrt{3}$ with Au coverage. The transition between $\sqrt{3}\times\sqrt{3}$ and 6x6 is an example of a commensurate-incommensurate transition. In fact, the Au/Si(111) system provides a rare opportunity to observe this type of phase transition on an atomic scale.

Specific scientific results are summarized as follows:

1) Surface reconstructions in the Au/Si(111) system

Gold is known to reconstruct the Si(111) surface, forming 5x1, $\sqrt{3}\times\sqrt{3}$, and 6x6 structures with increasing Au coverage up to 2 monolayers (ML). We have imaged all three surface phases. Furthermore, we have discovered that the $\sqrt{3}\times\sqrt{3}$ phase does not show long-range order, and that the transition from the $\sqrt{3}\times\sqrt{3}$ to the 6x6 phase is unique in several respects.

For the 5x1 structure, our results show that the basic surface unit cell is actually 5x2, and that the phase of the two unit cell periodicity is random between rows, thus breaking any long range 5x2 order. The structure is considerably more complex than that proposed in previous work on this surface. A significant density of bright features are scattered across the surface (about 1/40 ML), protruding from an otherwise fairly flat surface profile. These bright features always lie at a specific site in the 5x1 unit cell so that their distribution across the surface exhibits preferred relative spacings while having no long range order.

As the Au coverage increases, the next reconstruction that occurs is the $\sqrt{3}\times\sqrt{3}$ phase, which is visible in the low energy electron diffraction (LEED) pattern at between 0.6 and 1.0 ML. Previous studies have suggested that this phase evolves as a function of Au coverage, finally changing to the 6x6 phase at above 1 ML. Our STM studies reveal the true nature of this phase transition. The long range order of the $\sqrt{3}\times\sqrt{3}$ structure is always broken into sub-100Å domains by a series of serpentine domain walls. Each domain wall is a dislocation with a Burger's vector of one bulk lattice constant. The sizes of the domains contract as the coverage increases above

0.6 ML. At 1 ML, the surface structure is entirely 6x6. The 6x6 structure can in fact be described in terms of an array of dislocation loops encircling small sub-unit cells of $\sqrt{3}\times\sqrt{3}$ periodicity.

The unique aspect of the $\sqrt{3}\times\sqrt{3}$ to 6x6 phase transition is the fact that the $\sqrt{3}\times\sqrt{3}$ phase evolves with coverage, accommodating a range of Au densities by varying the density of the domain walls. In most other cases, a change in metal coverage results in a change of the relative population of surface phases, with each phase having a different and fixed metal atom density. For example, the transitions between the 7x7 to 5x1, and the 5x1 to $\sqrt{3}\times\sqrt{3}$ phases in the Au:Si(111) system follow this simple behavior.

2) The behavior of metals on the Si(100) surface at room temperature.

We have studied the initial stages of room temperature (RT) growth on Si(100) for Al, In, and Sn. At very low coverages, we have found that the surface mobility of these metals is sufficiently high at RT that the metal atoms arrange themselves into rows lying perpendicular to the underlying Si dimer rows. This is similar to the previously observed behavior of Ga on Si(100). The adsorption site appears to be the same in each case; the metal atoms are arranged as dimers lying over the trenches between the substrate Si dimer rows. As the coverage is increased, the metal configuration evolves from isolated, well-spaced rows, to areas of local 2x3 and 2x2 structure, to a surface entirely terminated by a 2x2 array of metal dimers at 0.5 ML. Sn differs slightly from the group III metals in that the 2x2 phase is not as well ordered.

The fact that the growth mode at low coverages is similar for all three metals suggests that this behavior is to some extent characteristic of the Si(100) surface. To test this hypothesis, we also examined the growth of Ag, Au and Sb at room temperature In all of these cases, the behavior was quite different, showing that one dimensional row growth is not a universal phenomenon. Ag was extremely mobile on the surface to the extent that it formed large two dimensional islands at even the lowest coverages studied. In a few areas, some tendency for the edges of the Ag islands to align either parallel or perpendicular to the Si dimer rows was seen. The mobility of both Au and Sb appeared to be very small, and low coverages of these adsorbates formed small, uncorrelated protrusions on the surface.

3) Metal Induced reconstructions of the In:Si(100) and Sn:Si(100) surfaces.

Although Al, In, Ga, and Sn seem to behave similarly at room temperature, all forming a 2x2 phase at 0.5 ML, each metal induces completely different reconstructions at higher temperatures. We have studied both the In and Sn:Si(100) systems. At this writing, the Sn data has been analyzed to only a limited extent, and will be described briefly. We will report in more detail on the In:Si(100) system.

Indium is known to induce two reconstructions: a 2x2 phase at low temperatures, and a higher temperature 4x3 phase. The 2x2 phase has already been described in the previous section. We have studied the evolution of the 4x3 phase with In coverage up to 0.5 ML, at which point the surface is entirely covered by 4x3. Diffraction experiments done elsewhere have shown that at still higher coverages, the Si surface becomes faceted, or the excess In forms three dimensional islands.

The separation between the low and the high temperature regimes for In is at about 150°C. At the higher temperatures, low coverages of In form isolated "bow tie" structures which contain approximately six In atoms each. It is difficult to assign a model for thes. structures because of a strong asymmetry in their appearance in unfilled and filled electronic states images. Empty state images of a bow tie show two maxima separated by roughly two unit cells along the direction of the Si dimer rows. In the filled states images, there is one central maxima positioned between the two empty state maxima. As the coverage increases, these bow ties arrange into rows oriented parallel to the Si dimer rows, with an inter-row spacing of four unit cells. At 0.5 ML, the bow ties are three unit cells apart along these rows, thus forming the 4x3 phase. The fact that the step distribution of the Si substrate is changed after annealing In on the surface, even in areas not covered by In at low coverage, suggests that Si displacement occurs during the formation of the 4x3 phase. There is also evidence that the In 4x3 phase "unzips" the underlying Si dimerzation, unlike the lower temperature 2x2 phase.

Previous diffraction studies of the Sn:Si(100) system have shown that there are many different reconstructions that arise as a function of coverage up to 1.5 ML. We have successfully imaged all but one of the phases previously known to exist. Furthermore, the STM images show

that the surface structure exhibits complex short range order that is not reflected in the LEED results. The behavior up to 1 ML can be summarized as follows: in this coverage range most of the surface atoms are bonded as dimers, just as for the clean Si(100) surface. The Sn atoms would then appear to be moving into substitutional sites. We find that once a significant percentage of the surface atoms are Sn, the dimers become strongly buckled and this buckling occurs in or out of phase for adjacent rows, resulting in various chain-like structures. At coverages above 0.5 ML, the dimers are periodically disrupted by one unit cell wide trenches oriented perpendicular to the dimer rows and spaced at relatively even intervals. The periodicity of these trenches can be sufficiently strong that satellite dots are visible in the LEED pattern, even when the structure of the dimer rows between the trenches is often insufficiently ordered to contribute to the diffraction pattern. Different combinations of the buckled dimers and the trench separations can result in a variety of local orderings, including 6×4, 5×4, and c(8×4). At certain coverages, some of these phases are sufficiently well ordered to be seen by LEED as well as by STM.

4) The Sb-terminated Si(100) surface

Antimony is an important dopant material used in Si molecular beam epitaxy. Studies have shown that Sb segregates to the surface under certain growth conditions, and that it is possible to grow a single monolayer of Sb on the surface. This layer can pull the surface Fermi level above the conduction band, resulting in a degenerate doping condition. The Sb-terminated Si(100) surface is then an extreme example of an abrupt doping profile, and raises the interesting prospect of being able to grow and to study single monolayer sheets of dopant atoms.

There is comparatively little information about the atomic structure of the Sb-terminated Si(100) surface. It is likely that the structure is similar to As:Si(100) where previous studies, including STM work, all support a model of symmetric As dimers. For Sb:Si(100), previous electron diffraction and STM results produced elsewhere have indicated imperfect 2×1 order, and a simple Sb dimer termination of the surface was not observed. These earlier studies used a growth temperature of 375°C, which we found to be insufficient to produce an ordered surface. Our surfaces were annealed to 540°C.

We have used STM to study the Sb-terminated Si(100) surface at coverages near 1 ML. The images clearly show that the surface is terminated in a dimer structure similar to that seen for As:Si(100). However, the surface is considerably less ordered than either clean Si(100) or As:Si(100). The long-range 2×1 order is broken up by a high density of defects, including voids and anti-phase domain boundaries, which account for the diffuseness of the half-order dots in the 2×1 LEED pattern. Images taken on single-domain Si(100) substrates demonstrate that the Sb grows as an additional layer of dimers, rather than substituting for the topmost layer of Si dimers.